2-Ethylhexyl 2-phenoxybutyrate

Inchi: InChI=1S/C18H28O3/c1-4-7-11-15(5-2)14-20-18(19)17(6-3)21-16-12-9-8-10-13-16/h8-10
InchiKey: OPTLGOZUDPLGKB-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCC(CC)COC(=O)C(CC)Oc1ccccc1
Mol. weight [g/mol]: 292.41

Physical Properties

Property code	Value	Unit	Source
gf	-130.71	kJ/mol	Joback Method
hf	-565.90	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	68.73	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.604		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1871.00		NIST Webbook
tb	735.75	K	Joback Method
tc	932.65	K	Joback Method
tf	383.43	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.74	J/mol×K	735.75	Joback Method
cpg	759.64	J/mol×K	768.57	Joback Method
cpg	776.46	J/mol×K	801.38	Joback Method
cpg	792.22	J/mol×K	834.20	Joback Method
cpg	806.95	J/mol×K	867.01	Joback Method
cpg	820.67	J/mol×K	899.83	Joback Method
cpg	833.40	J/mol×K	932.65	Joback Method
dvisc	0.0016164	Pa×s	383.43	Joback Method
dvisc	0.0006558	Pa×s	442.15	Joback Method

dvisc	0.0003287	Pa×s	500.87	Joback Method
dvisc	0.0001905	Pa×s	559.59	Joback Method
dvisc	0.0001224	Pa×s	618.31	Joback Method
dvisc	0.0000849	Pa×s	677.03	Joback Method
dvisc	0.0000625	Pa×s	735.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540306&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume